



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:33 PM GMT

PDB ID : 2O7C  
Title : Crystal structure of L-methionine-lyase from Pseudomonas  
Authors : Misaki, S.; Takimoto, A.; Takakura, T.; Yoshioka, T.; Yamashita, M.; Tamura, T.; Tanaka, H.; Inagaki, K.  
Deposited on : 2006-12-10  
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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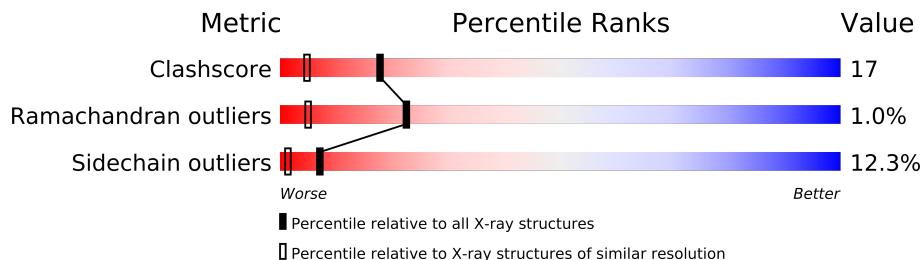
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
1	C	398	
1	D	398	

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12783 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	B	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	C	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	D	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total	O	0	0
			165	165		
3	B	172	Total	O	0	0
			172	172		
3	C	197	Total	O	0	0
			197	197		
3	D	185	Total	O	0	0
			185	185		

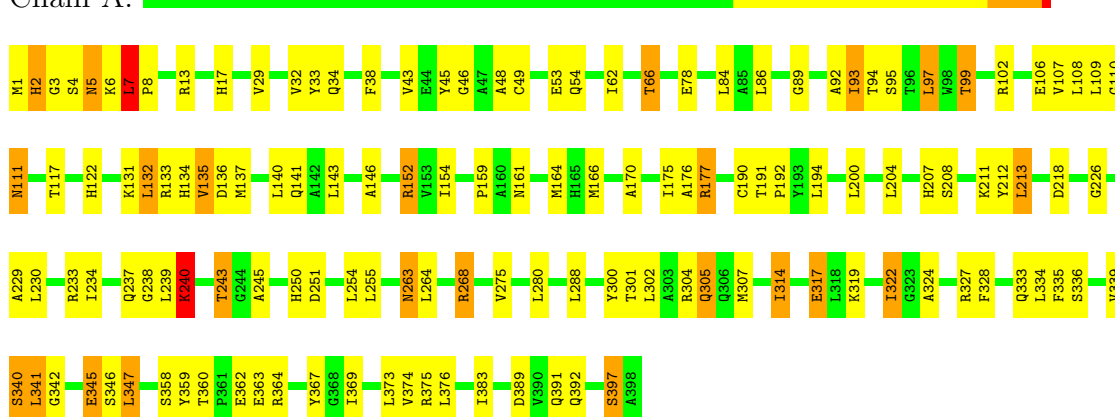
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

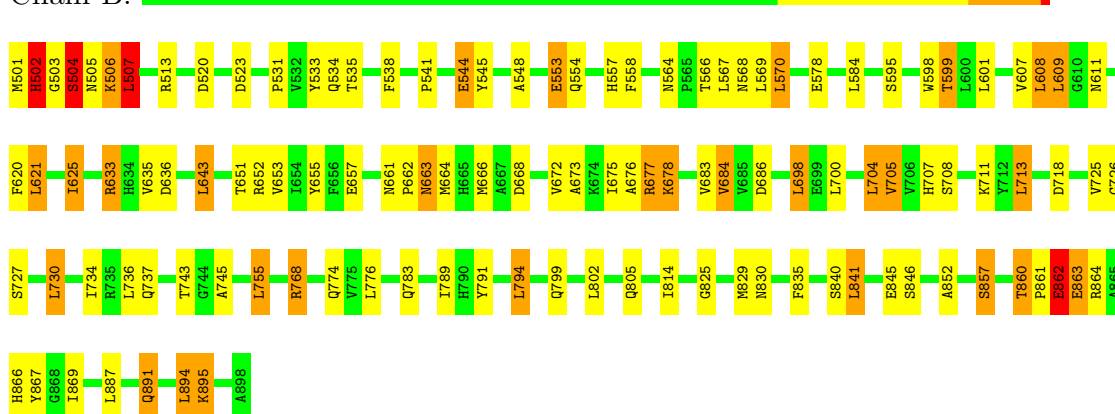
#### • Molecule 1: Methionine gamma-lyase

Chain A:



#### • Molecule 1: Methionine gamma-lyase

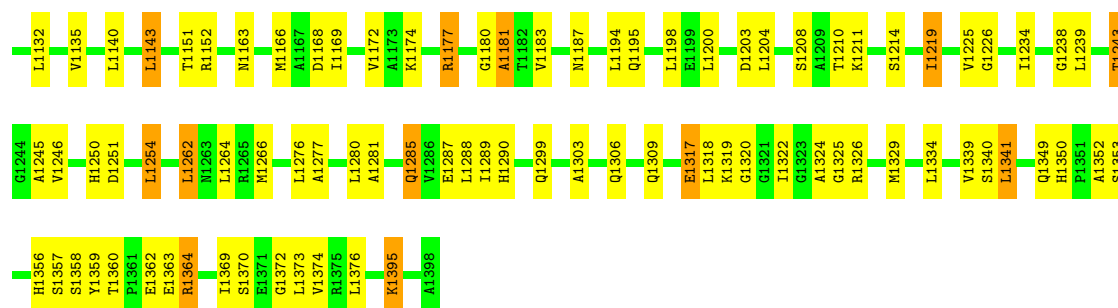
Chain B:



#### • Molecule 1: Methionine gamma-lyase

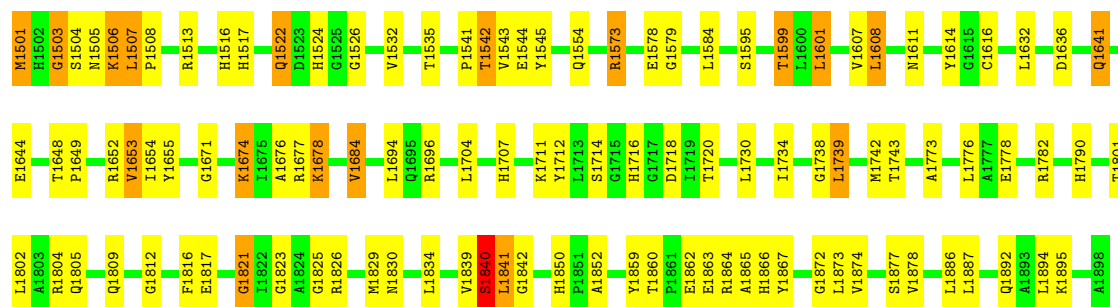
Chain C:





- Molecule 1: Methionine gamma-lyase

Chain D:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.13Å 133.13Å 215.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.36	0/3051	0.61	1/4139 (0.0%)
1	B	0.36	0/3051	0.63	1/4139 (0.0%)
1	C	0.36	0/3051	0.61	1/4139 (0.0%)
1	D	0.36	0/3051	0.61	1/4139 (0.0%)
All	All	0.36	0/12204	0.62	4/16556 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	SER	N-CA-C	-5.63	95.79	111.00
1	B	708	SER	N-CA-C	-5.39	96.46	111.00
1	D	1877	SER	N-CA-C	-5.38	96.46	111.00
1	C	1208	SER	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3011	0	2973	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3011	0	2969	102	0
1	C	3011	0	2969	120	0
1	D	3011	0	2970	95	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	165	0	0	8	0
3	B	172	0	0	8	0
3	C	197	0	0	9	0
3	D	185	0	0	5	0
All	All	12783	0	11881	411	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (411) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:VAL:HB	1:D:1535:THR:HG22	1.15	1.07
1:B:663:ASN:HD22	1:B:663:ASN:H	1.07	1.01
1:C:1003:GLY:HA2	1:C:1013:ARG:HG2	1.44	0.97
1:D:1507:LEU:HB2	1:D:1508:PRO:HD3	1.50	0.94
1:B:533:TYR:HB3	3:B:993:HOH:O	1.68	0.93
1:D:1542:THR:HG22	1:D:1545:TYR:H	1.41	0.86
1:C:1061:ARG:NH2	1:D:1616:CYS:SG	2.50	0.84
1:C:1043:VAL:H	1:D:1830:ASN:HD21	1.24	0.84
1:C:1061:ARG:HG3	1:C:1246:VAL:CG2	2.07	0.83
1:C:1211:LLP:HD3	1:C:1341:LEU:HD13	1.58	0.83
1:A:43:VAL:H	1:B:830:ASN:HD21	1.23	0.83
1:A:29:VAL:HB	1:D:1535:THR:CG2	2.07	0.82
1:B:663:ASN:ND2	1:B:663:ASN:H	1.78	0.81
1:C:1219:ILE:HD11	1:C:1251:ASP:HA	1.64	0.80
1:B:666:MET:H	1:B:799:GLN:HE22	1.29	0.80
1:B:663:ASN:HD22	1:B:663:ASN:N	1.78	0.79
1:C:1276:LEU:HB2	3:C:1585:HOH:O	1.81	0.79
1:C:1166:MET:H	1:C:1299:GLN:HE22	1.30	0.78
3:A:526:HOH:O	1:D:1522:GLN:HG3	1.81	0.78
1:B:863:GLU:HA	1:B:866:HIS:HB3	1.65	0.78
1:B:860:THR:C	1:B:862:GLU:H	1.86	0.78
1:C:1243:THR:OG1	1:D:1743:THR:HA	1.83	0.77
1:C:1095:SER:O	1:C:1099:THR:HG23	1.86	0.75
1:B:535:THR:HG22	3:B:993:HOH:O	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:33:TYR:H	1:A:66:THR:HG21	1.52	0.74
1:A:93:ILE:HG13	1:A:94:THR:N	2.01	0.74
1:B:894:LEU:HB3	1:B:895:LYS:HZ2	1.53	0.74
1:A:239:LEU:O	1:A:240:LYS:HB3	1.88	0.73
1:A:99:THR:HG21	1:A:234:ILE:HA	1.70	0.73
1:A:33:TYR:H	1:A:66:THR:CG2	2.01	0.73
1:C:1277:ALA:HB3	3:C:1403:HOH:O	1.87	0.73
1:D:1501:MET:N	1:D:1516:HIS:HB3	2.04	0.72
1:A:110:GLY:O	1:A:134:HIS:HD2	1.72	0.72
1:B:502:HIS:HB2	1:D:1834:LEU:HD13	1.70	0.72
1:A:3:GLY:O	1:A:13:ARG:HG2	1.90	0.72
1:D:1812:GLY:O	1:D:1878:VAL:HG12	1.89	0.71
1:C:1219:ILE:HD12	1:C:1254:LEU:HD23	1.73	0.71
1:A:5:ASN:N	1:A:5:ASN:HD22	1.89	0.71
1:C:1061:ARG:HG3	1:C:1246:VAL:HG21	1.71	0.71
1:A:302:LEU:HA	1:A:305:GLN:HG3	1.73	0.70
1:C:1093:ILE:HG13	1:C:1094:THR:N	2.06	0.70
1:C:1276:LEU:HD22	3:C:1585:HOH:O	1.92	0.70
1:D:1773:ALA:HB2	1:D:1878:VAL:HG11	1.74	0.69
1:D:1738:GLY:O	1:D:1742:MET:O	2.11	0.69
1:B:891:GLN:HE21	1:B:891:GLN:HA	1.57	0.69
1:A:111:ASN:ND2	1:A:136:ASP:HA	2.07	0.69
1:D:1595:SER:O	1:D:1599:THR:HG23	1.92	0.69
1:B:620:PHE:CZ	1:B:625:ILE:HG12	2.28	0.69
1:D:1504:SER:HB2	1:D:1517:HIS:CD2	2.27	0.68
1:A:2:HIS:HB2	1:C:1334:LEU:HD13	1.74	0.68
1:C:1166:MET:CE	1:C:1303:ALA:HA	2.24	0.68
1:B:666:MET:H	1:B:799:GLN:NE2	1.90	0.67
1:C:1329:MET:HE3	1:C:1374:VAL:HB	1.76	0.67
1:B:599:THR:HG21	1:B:734:ILE:HA	1.75	0.67
1:D:1542:THR:HG22	1:D:1545:TYR:N	2.10	0.67
1:C:1001:MET:HA	1:C:1008:PRO:HG3	1.77	0.67
1:C:1114:TYR:HB3	1:C:1117:THR:CG2	2.25	0.66
1:C:1114:TYR:HB3	1:C:1117:THR:HG23	1.76	0.66
1:A:95:SER:O	1:A:99:THR:HG23	1.96	0.66
1:C:1370:SER:HB3	1:C:1373:LEU:HB2	1.77	0.65
1:C:1276:LEU:O	1:C:1280:LEU:HD23	1.95	0.65
1:D:1542:THR:HG23	1:D:1544:GLU:H	1.62	0.65
1:C:1121:LEU:HD23	1:C:1125:ILE:CD1	2.27	0.65
3:C:1444:HOH:O	1:D:1720:THR:HG23	1.97	0.65
1:C:1166:MET:HE1	1:C:1303:ALA:HA	1.78	0.65
1:B:507:LEU:O	1:B:507:LEU:HD23	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1507:LEU:HB2	1:D:1508:PRO:CD	2.26	0.65
1:C:1169:ILE:H	1:C:1306:GLN:HE22	1.45	0.65
1:B:774:GLN:HG2	3:B:909:HOH:O	1.97	0.65
1:C:1121:LEU:HA	1:C:1125:ILE:HD12	1.77	0.64
1:D:1517:HIS:O	1:D:1573:ARG:HD3	1.97	0.64
1:B:860:THR:O	1:B:862:GLU:N	2.30	0.64
1:D:1542:THR:CG2	1:D:1545:TYR:H	2.11	0.64
1:D:1711:LLP:HD3	1:D:1841:LEU:HG	1.80	0.64
3:A:427:HOH:O	1:D:1535:THR:HG23	1.97	0.63
1:B:894:LEU:HB3	1:B:895:LYS:NZ	2.12	0.63
1:D:1542:THR:HG23	1:D:1544:GLU:N	2.13	0.63
1:C:1099:THR:HG21	1:C:1234:ILE:HA	1.80	0.62
1:A:263:ASN:H	1:A:263:ASN:HD22	1.45	0.62
1:C:1089:GLY:O	1:C:1093:ILE:HG23	2.00	0.62
1:A:29:VAL:CB	1:D:1535:THR:HG22	2.10	0.61
1:C:1117:THR:HG21	3:C:1460:HOH:O	2.00	0.61
1:A:108:LEU:HD23	1:A:133:ARG:HB3	1.80	0.61
1:D:1504:SER:HA	1:D:1513:ARG:HD3	1.84	0.60
1:A:109:LEU:HB2	1:A:134:HIS:CD2	2.36	0.60
1:A:29:VAL:O	1:D:1535:THR:HG21	1.99	0.60
1:A:250:HIS:HD2	1:A:251:ASP:OD2	1.84	0.60
1:B:867:TYR:HB3	1:B:869:ILE:CD1	2.31	0.60
1:A:239:LEU:O	1:A:240:LYS:CB	2.49	0.60
1:D:1599:THR:HG21	1:D:1734:ILE:HA	1.83	0.60
1:C:1135:VAL:HG21	1:C:1143:LEU:HD23	1.83	0.60
1:D:1504:SER:C	1:D:1506:LYS:H	2.04	0.59
1:C:1219:ILE:CD1	1:C:1254:LEU:HD23	2.32	0.59
1:A:345:GLU:HG3	1:C:1028:LEU:HD11	1.84	0.59
1:C:1098:TRP:CZ3	1:C:1125:ILE:HG23	2.38	0.59
1:C:1243:THR:CG2	1:C:1245:ALA:H	2.15	0.59
1:A:111:ASN:HD22	1:A:136:ASP:HA	1.67	0.59
1:B:598:TRP:CZ3	1:B:625:ILE:HG23	2.37	0.58
1:D:1524:HIS:HD2	3:D:2034:HOH:O	1.85	0.58
1:A:339:VAL:HG22	3:B:936:HOH:O	2.04	0.58
1:C:1121:LEU:HA	1:C:1125:ILE:CD1	2.33	0.58
1:B:704:LEU:HD12	1:B:726:GLY:HA3	1.85	0.58
1:B:655:TYR:CD1	1:B:684:VAL:HG22	2.39	0.58
1:A:108:LEU:HD21	1:A:133:ARG:HH21	1.68	0.58
1:B:601:LEU:HD21	1:B:653:VAL:HG13	1.86	0.58
1:A:211:LLP:HD3	1:A:341:LEU:HG	1.84	0.58
1:B:863:GLU:OE2	1:B:867:TYR:HB2	2.04	0.58
1:D:1595:SER:O	1:D:1599:THR:CG2	2.51	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1860:THR:H	1:D:1863:GLU:HB2	1.69	0.58
1:C:1166:MET:H	1:C:1299:GLN:NE2	1.99	0.57
1:B:727:SER:OG	1:B:730:LEU:HB2	2.05	0.57
1:B:595:SER:O	1:B:599:THR:CG2	2.53	0.57
1:A:143:LEU:HD23	1:A:175:ILE:HD12	1.87	0.57
1:A:108:LEU:CD2	1:A:133:ARG:HB3	2.35	0.56
1:B:599:THR:HB	1:B:737:GLN:HG2	1.86	0.56
1:A:48:ALA:CB	1:A:54:GLN:HB2	2.35	0.56
1:B:608:LEU:HD22	1:B:651:THR:HG21	1.86	0.56
1:A:389:ASP:O	1:A:392:GLN:HG3	2.05	0.56
1:A:359:TYR:HB2	1:A:364:ARG:HG3	1.87	0.56
1:A:288:LEU:HB3	1:A:317:GLU:HG3	1.87	0.56
1:C:1360:THR:OG1	1:C:1362:GLU:HG2	2.06	0.56
1:B:867:TYR:HB3	1:B:869:ILE:HD11	1.88	0.56
1:B:768:ARG:NH1	3:B:988:HOH:O	2.36	0.56
1:A:322:ILE:HG13	3:A:559:HOH:O	2.06	0.56
1:A:3:GLY:HA2	1:A:13:ARG:HG2	1.88	0.56
1:C:1290:HIS:HD2	3:C:1466:HOH:O	1.88	0.56
1:A:110:GLY:O	1:A:134:HIS:CD2	2.57	0.55
1:B:668:ASP:O	1:B:672:VAL:HG13	2.06	0.55
1:A:154:ILE:HD12	1:A:176:ALA:HB2	1.88	0.55
1:B:860:THR:C	1:B:862:GLU:N	2.54	0.55
1:C:1285:GLN:HE21	1:C:1285:GLN:H	1.54	0.55
1:C:1262:LEU:HD22	1:C:1266:MET:HG2	1.89	0.55
1:D:1504:SER:C	1:D:1506:LYS:N	2.59	0.55
1:B:676:ALA:HB3	1:B:677:ARG:HH21	1.72	0.55
1:A:327:ARG:NH2	1:A:397:SER:O	2.40	0.55
1:C:1003:GLY:CA	1:C:1013:ARG:HG2	2.28	0.55
1:B:570:LEU:HD21	1:B:755:LEU:HD13	1.88	0.55
1:C:1108:LEU:HD22	1:C:1151:THR:HG21	1.88	0.55
1:A:78:GLU:HG2	1:A:192:PRO:HB3	1.88	0.54
1:B:548:ALA:CB	1:B:554:GLN:HB2	2.37	0.54
1:C:1204:LEU:HD23	1:C:1226:GLY:HA3	1.87	0.54
1:D:1839:VAL:O	1:D:1840:SER:CB	2.55	0.54
1:B:675:ILE:HA	1:B:678:LYS:HE3	1.90	0.54
1:C:1091:GLY:HA2	1:D:1743:THR:O	2.08	0.54
1:C:1002:HIS:O	1:C:1017:HIS:HA	2.07	0.54
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.91	0.54
1:B:607:VAL:HG22	1:B:609:LEU:HD13	1.89	0.54
1:A:300:TYR:O	1:A:304:ARG:HG2	2.08	0.53
1:C:1320:GLY:HA3	1:C:1324:ALA:HB2	1.90	0.53
1:A:32:VAL:HB	1:D:1532:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1011:ALA:O	1:C:1015:ILE:HG23	2.09	0.53
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.61	0.53
1:C:1194:LEU:HD22	1:C:1309:GLN:HB2	1.90	0.53
1:A:8:PRO:O	1:A:13:ARG:HD3	2.09	0.53
1:C:1047:ALA:HA	1:C:1050:PHE:HD1	1.73	0.53
1:D:1504:SER:O	1:D:1507:LEU:HG	2.08	0.53
1:D:1694:LEU:HD22	1:D:1809:GLN:HB2	1.91	0.53
1:D:1677:ARG:NE	1:D:1677:ARG:HA	2.23	0.53
1:D:1778:GLU:O	1:D:1782:ARG:HG3	2.09	0.53
1:B:860:THR:OG1	1:B:862:GLU:HG2	2.09	0.52
1:C:1169:ILE:H	1:C:1306:GLN:NE2	2.07	0.52
1:B:548:ALA:HB1	1:B:554:GLN:HB2	1.90	0.52
1:A:135:VAL:HG23	1:A:137:MET:CE	2.39	0.52
1:A:339:VAL:O	1:A:340:SER:CB	2.58	0.52
1:A:48:ALA:HB1	1:A:54:GLN:HB2	1.90	0.52
1:D:1696:ARG:NH2	3:D:2043:HOH:O	2.42	0.52
1:D:1816:PHE:CE1	1:D:1874:VAL:HG22	2.44	0.52
1:B:608:LEU:HD22	1:B:651:THR:CG2	2.39	0.52
1:D:1507:LEU:CB	1:D:1508:PRO:HD3	2.32	0.52
1:A:238:GLY:O	1:A:243:THR:HB	2.10	0.52
1:B:502:HIS:CB	1:D:1834:LEU:HD13	2.39	0.52
1:C:1120:PHE:CZ	1:C:1125:ILE:HG12	2.44	0.52
1:D:1601:LEU:HD21	1:D:1607:VAL:HG21	1.90	0.52
1:C:1168:ASP:O	1:C:1172:VAL:HG13	2.09	0.52
1:C:1395:LYS:HD3	1:C:1395:LYS:N	2.25	0.52
1:D:1578:GLU:OE1	1:D:1707:HIS:HE1	1.92	0.52
1:B:863:GLU:HG3	1:B:863:GLU:O	2.09	0.52
1:C:1250:HIS:HD2	1:C:1251:ASP:OD2	1.93	0.52
1:D:1821:GLY:HA2	1:D:1872:GLY:HA3	1.91	0.52
1:B:663:ASN:ND2	1:B:663:ASN:N	2.45	0.52
1:B:743:THR:HG22	1:B:745:ALA:HB2	1.92	0.52
1:B:862:GLU:CG	1:B:863:GLU:H	2.21	0.51
1:A:229:ALA:O	1:A:233:ARG:HG3	2.11	0.51
1:A:3:GLY:HA2	1:A:13:ARG:CG	2.41	0.51
1:A:34:GLN:HG3	1:B:718:ASP:O	2.11	0.51
1:B:538:PHE:HB2	1:B:558:PHE:HA	1.92	0.51
1:D:1641:GLN:NE2	1:D:1641:GLN:H	2.09	0.51
1:C:1114:TYR:CE2	1:C:1116:CYS:HB2	2.45	0.51
1:B:705:VAL:HG23	1:B:725:VAL:HB	1.93	0.51
1:D:1865:ALA:C	1:D:1867:TYR:H	2.14	0.50
1:B:768:ARG:NH2	3:B:1072:HOH:O	2.39	0.50
1:C:1166:MET:HE2	1:C:1303:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:HIS:NE2	1:A:134:HIS:HE1	2.09	0.50
1:A:133:ARG:NH2	1:A:146:ALA:O	2.45	0.50
1:C:1285:GLN:H	1:C:1285:GLN:NE2	2.09	0.50
1:B:501:MET:HA	1:B:501:MET:CE	2.42	0.50
1:C:1287:GLU:HB2	1:C:1319:LYS:HG2	1.92	0.50
1:B:673:ALA:O	1:B:677:ARG:NE	2.45	0.50
1:B:705:VAL:CG2	1:B:725:VAL:HB	2.42	0.50
1:B:502:HIS:HB2	1:D:1834:LEU:CD1	2.41	0.50
1:B:611:ASN:OD1	1:B:636:ASP:HA	2.11	0.50
1:B:891:GLN:CA	1:B:891:GLN:HE21	2.23	0.50
1:C:1200:LEU:HD11	1:C:1306:GLN:HG2	1.94	0.50
1:B:557:HIS:HE1	1:B:568:ASN:ND2	2.09	0.50
1:D:1716:HIS:HB2	3:D:2059:HOH:O	2.11	0.50
1:C:1349:GLN:NE2	3:C:1532:HOH:O	2.44	0.50
1:D:1648:THR:HB	1:D:1649:PRO:HD2	1.94	0.50
1:A:360:THR:OG1	1:A:363:GLU:HG3	2.12	0.50
1:A:213:LEU:HB3	1:A:255:LEU:HD11	1.93	0.49
1:C:1243:THR:HG23	1:C:1245:ALA:H	1.77	0.49
1:C:1243:THR:HG23	1:C:1245:ALA:CB	2.42	0.49
1:D:1578:GLU:OE1	1:D:1707:HIS:CE1	2.66	0.49
1:B:711:LLP:HD3	1:B:841:LEU:HG	1.94	0.49
1:D:1541:PRO:HD2	1:D:1545:TYR:CD1	2.47	0.49
1:D:1601:LEU:HD11	1:D:1653:VAL:HG13	1.94	0.49
1:D:1504:SER:CB	1:D:1517:HIS:CD2	2.94	0.49
1:A:194:LEU:O	1:A:307:MET:HA	2.13	0.48
1:D:1790:HIS:HE1	1:D:1817:GLU:OE1	1.96	0.48
1:C:1061:ARG:HG3	1:C:1246:VAL:HG22	1.91	0.48
1:A:161:ASN:HD21	1:A:375:ARG:HD2	1.76	0.48
1:C:1219:ILE:HD13	1:C:1254:LEU:HB3	1.94	0.48
1:B:595:SER:O	1:B:599:THR:HG23	2.13	0.48
1:B:676:ALA:CB	1:B:677:ARG:HH21	2.26	0.48
1:A:32:VAL:HB	1:D:1532:VAL:CG1	2.44	0.48
1:D:1825:GLY:O	1:D:1829:MET:HG2	2.13	0.48
1:B:507:LEU:HD22	3:B:1022:HOH:O	2.13	0.48
1:A:345:GLU:HG3	1:C:1028:LEU:CD1	2.44	0.48
1:D:1860:THR:HG23	1:D:1863:GLU:OE2	2.13	0.48
1:B:503:GLY:O	1:B:513:ARG:HG2	2.14	0.48
1:A:367:TYR:HB3	1:A:369:ILE:HD12	1.96	0.48
1:B:677:ARG:N	1:B:677:ARG:HE	2.12	0.48
3:C:1434:HOH:O	1:D:1839:VAL:HG22	2.13	0.48
1:D:1859:TYR:HB2	1:D:1864:ARG:HG3	1.94	0.48
1:C:1211:LLP:HD3	1:C:1341:LEU:CD1	2.38	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:ALA:HB1	1:A:53:GLU:HG3	1.96	0.47
1:C:1364:ARG:HG2	1:C:1369:ILE:HB	1.96	0.47
1:B:783:GLN:HG3	1:B:894:LEU:CD2	2.45	0.47
1:D:1654:ILE:HD12	1:D:1676:ALA:HB2	1.96	0.47
1:D:1503:GLY:C	1:D:1517:HIS:HD2	2.17	0.47
1:C:1339:VAL:O	1:C:1340:SER:HB3	2.13	0.47
1:C:1057:HIS:HE1	1:C:1068:ASN:HD21	1.62	0.47
1:D:1584:LEU:HD11	1:D:1739:LEU:HD12	1.97	0.47
1:A:43:VAL:HG22	1:B:830:ASN:HD21	1.79	0.47
1:A:95:SER:OG	1:A:243:THR:HG21	2.14	0.47
1:B:608:LEU:HD12	1:B:633:ARG:HB3	1.97	0.47
1:C:1108:LEU:HD22	1:C:1151:THR:CG2	2.45	0.47
1:D:1714:SER:OG	3:D:2059:HOH:O	2.21	0.47
1:C:1180:GLY:O	1:C:1181:ALA:O	2.33	0.47
1:D:1671:GLY:O	1:D:1674:LYS:HE2	2.15	0.47
1:C:1187:ASN:ND2	1:C:1195:GLN:HE21	2.12	0.47
1:A:328:PHE:HB2	1:A:397:SER:HB2	1.97	0.47
1:C:1177:ARG:NH2	1:C:1203:ASP:OD1	2.48	0.47
1:A:3:GLY:HA2	1:A:13:ARG:HA	1.96	0.46
1:A:190:CYS:O	1:A:194:LEU:HB2	2.14	0.46
1:C:1198:LEU:HD11	1:C:1225:VAL:HG12	1.97	0.46
1:B:657:GLU:HG2	1:B:686:ASP:HB3	1.96	0.46
1:A:301:THR:O	1:A:305:GLN:HG2	2.14	0.46
1:C:1352:ALA:O	1:C:1357:SER:HA	2.16	0.46
1:A:218:ASP:O	1:B:534:GLN:HG3	2.16	0.46
1:B:661:ASN:HB3	1:B:662:PRO:HA	1.97	0.46
1:B:698:LEU:HB2	3:B:975:HOH:O	2.15	0.46
1:A:164:MET:O	1:A:166:MET:HE2	2.15	0.46
1:C:1243:THR:HG22	1:C:1245:ALA:H	1.80	0.46
1:A:62:ILE:HG13	1:A:240:LYS:HD3	1.98	0.46
1:B:544:GLU:HG2	1:B:544:GLU:H	1.39	0.46
1:C:1318:LEU:HD12	1:C:1325:GLY:HA2	1.96	0.46
1:D:1614:TYR:CE2	1:D:1616:CYS:HB2	2.51	0.46
1:A:135:VAL:HG23	1:A:137:MET:HE2	1.97	0.46
1:C:1057:HIS:HE1	1:C:1068:ASN:ND2	2.14	0.46
1:A:345:GLU:HG2	1:A:345:GLU:H	1.49	0.46
1:C:1034:GLN:HG3	1:D:1718:ASP:O	2.16	0.46
1:D:1506:LYS:HE3	1:D:1579:GLY:HA2	1.98	0.46
1:D:1866:HIS:C	1:D:1867:TYR:HD1	2.19	0.46
1:B:564:ASN:ND2	1:B:566:THR:HB	2.30	0.46
1:C:1288:LEU:HB3	1:C:1317:GLU:HG3	1.98	0.46
1:D:1505:ASN:O	1:D:1506:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1114:TYR:HD2	1:C:1117:THR:HG22	1.81	0.46
1:B:621:LEU:HD13	1:B:625:ILE:HD11	1.98	0.46
1:A:159:PRO:HB3	1:A:166:MET:CE	2.46	0.45
1:C:1003:GLY:O	1:C:1008:PRO:HD2	2.17	0.45
1:A:3:GLY:O	1:A:17:HIS:HD2	1.98	0.45
1:A:170:ALA:HA	1:A:200:LEU:O	2.16	0.45
1:B:663:ASN:O	1:B:664:MET:HB2	2.17	0.45
1:B:564:ASN:ND2	1:B:566:THR:H	2.15	0.45
1:C:1003:GLY:O	1:C:1013:ARG:HD3	2.17	0.45
1:C:1243:THR:HG23	1:C:1245:ALA:HB2	1.98	0.45
1:B:564:ASN:HD22	1:B:567:LEU:H	1.65	0.45
1:B:578:GLU:OE2	1:B:707:HIS:CE1	2.70	0.45
1:A:2:HIS:CE1	1:A:5:ASN:HB2	2.52	0.45
1:C:1326:ARG:HG2	1:D:1543:VAL:HG11	1.99	0.45
1:B:864:ARG:HA	1:B:869:ILE:HD12	1.98	0.45
1:A:93:ILE:HD13	1:A:117:THR:HG23	1.98	0.45
1:D:1862:GLU:HB3	1:D:1866:HIS:NE2	2.32	0.45
1:C:1356:HIS:O	1:C:1359:TYR:HB2	2.16	0.44
1:B:852:ALA:HA	1:B:864:ARG:HD3	1.99	0.44
1:C:1238:GLY:O	1:C:1243:THR:HB	2.17	0.44
1:A:108:LEU:CD2	1:A:133:ARG:HD2	2.47	0.44
1:A:324:ALA:HA	1:A:327:ARG:NH2	2.32	0.44
1:A:212:TYR:CD1	1:A:342:GLY:HA2	2.53	0.44
1:A:89:GLY:O	1:A:93:ILE:HG23	2.17	0.44
1:A:46:GLY:O	1:A:49:CYS:HB2	2.18	0.44
1:A:335:PHE:CE1	1:A:346:SER:HB3	2.52	0.44
1:C:1219:ILE:CD1	1:C:1254:LEU:HB3	2.48	0.44
1:A:2:HIS:HB3	1:A:3:GLY:H	1.48	0.44
1:C:1046:GLY:O	1:C:1050:PHE:CD1	2.71	0.44
1:A:314:ILE:CG2	1:A:376:LEU:HB2	2.48	0.44
1:A:152:ARG:NH1	3:A:552:HOH:O	2.49	0.44
1:B:791:TYR:HB3	1:B:794:LEU:HD22	2.00	0.44
1:D:1601:LEU:HD21	1:D:1607:VAL:CG2	2.48	0.44
1:A:233:ARG:O	1:A:237:GLN:HB2	2.18	0.44
1:A:243:THR:HG23	1:A:245:ALA:H	1.83	0.43
1:C:1281:ALA:HA	1:C:1289:ILE:HD11	1.99	0.43
1:A:5:ASN:ND2	1:A:5:ASN:N	2.60	0.43
1:B:713:LEU:HB3	1:B:755:LEU:HD21	2.00	0.43
1:B:505:ASN:HA	1:B:513:ARG:HD2	2.00	0.43
1:D:1711:LLP:O3	1:D:1711:LLP:NZ	2.50	0.43
1:D:1866:HIS:ND1	1:D:1866:HIS:N	2.67	0.43
1:D:1801:THR:O	1:D:1805:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1006:LYS:HE2	1:C:1007:LEU:H	1.83	0.43
1:A:2:HIS:CG	1:A:5:ASN:HB2	2.53	0.43
1:C:1350:HIS:HD2	1:C:1373:LEU:O	2.02	0.43
1:A:66:THR:HB	3:A:508:HOH:O	2.18	0.43
1:A:336:SER:HB2	1:A:347:LEU:HD12	2.00	0.43
1:C:1341:LEU:HD13	1:C:1341:LEU:N	2.34	0.43
1:C:1243:THR:HG23	1:C:1245:ALA:N	2.34	0.43
1:C:1200:LEU:CD1	1:C:1306:GLN:HG2	2.49	0.43
1:A:99:THR:HG22	1:A:238:GLY:CA	2.49	0.43
1:C:1339:VAL:O	1:C:1340:SER:CB	2.67	0.43
1:D:1644:GLU:OE1	1:D:1678:LYS:HE3	2.19	0.43
1:B:677:ARG:NH2	1:B:683:VAL:HG23	2.33	0.42
1:C:1163:ASN:HB2	3:C:1580:HOH:O	2.19	0.42
1:B:553:GLU:H	1:B:553:GLU:HG2	1.67	0.42
1:C:1007:LEU:N	1:C:1008:PRO:HD3	2.35	0.42
1:A:322:ILE:H	1:A:322:ILE:HG13	1.49	0.42
1:A:359:TYR:N	1:A:359:TYR:CD1	2.87	0.42
1:D:1684:VAL:HA	1:D:1704:LEU:O	2.19	0.42
1:D:1850:HIS:NE2	1:D:1852:ALA:HB3	2.34	0.42
1:C:1210:THR:HG23	1:C:1219:ILE:O	2.19	0.42
1:C:1360:THR:H	1:C:1363:GLU:HB2	1.84	0.42
1:A:107:VAL:CG1	1:A:132:LEU:HD12	2.48	0.42
1:C:1276:LEU:O	1:C:1280:LEU:CD2	2.65	0.42
1:C:1004:SER:HB2	1:C:1017:HIS:HE1	1.85	0.42
1:D:1712:TYR:CE1	1:D:1842:GLY:HA2	2.55	0.42
1:B:743:THR:CG2	1:B:745:ALA:HB2	2.50	0.42
1:D:1865:ALA:C	1:D:1867:TYR:N	2.72	0.42
1:A:43:VAL:HG22	1:B:830:ASN:ND2	2.35	0.42
1:B:891:GLN:O	1:B:895:LYS:HD2	2.19	0.42
1:A:108:LEU:HD21	1:A:133:ARG:HD2	2.02	0.42
1:B:643:LEU:HD13	1:B:675:ILE:HG21	2.01	0.42
1:B:852:ALA:O	1:B:857:SER:HA	2.20	0.42
1:A:111:ASN:ND2	3:A:499:HOH:O	2.52	0.42
1:C:1125:ILE:H	1:C:1125:ILE:HG13	1.32	0.42
1:B:506:LYS:H	1:B:513:ARG:CZ	2.31	0.42
1:B:531:PRO:HB2	1:C:1031:PRO:HB2	2.00	0.42
1:D:1862:GLU:CD	1:D:1862:GLU:H	2.22	0.42
1:D:1599:THR:HG22	1:D:1738:GLY:CA	2.50	0.42
1:B:835:PHE:CE2	1:B:846:SER:HB3	2.55	0.42
1:A:177:ARG:HD2	3:A:525:HOH:O	2.20	0.42
1:D:1542:THR:CG2	1:D:1545:TYR:N	2.79	0.41
1:C:1095:SER:OG	1:C:1243:THR:HG21	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:HIS:C	1:A:4:SER:H	2.24	0.41
1:A:211:LLP:NZ	1:A:211:LLP:O3	2.53	0.41
1:A:191:THR:HB	1:A:192:PRO:HD2	2.02	0.41
1:C:1102:ARG:HD3	1:C:1102:ARG:HA	1.90	0.41
1:B:635:VAL:HG11	1:B:643:LEU:HA	2.01	0.41
1:C:1353:SER:C	1:C:1357:SER:HB2	2.41	0.41
1:D:1611:ASN:HD21	1:D:1636:ASP:HB2	1.85	0.41
1:A:102:ARG:HD3	1:A:102:ARG:HA	1.88	0.41
1:A:3:GLY:CA	1:A:13:ARG:HG2	2.50	0.41
1:A:268:ARG:HB2	1:A:268:ARG:NH1	2.35	0.41
1:C:1219:ILE:HG12	1:C:1251:ASP:HB3	2.01	0.41
1:B:704:LEU:HD13	1:B:730:LEU:HD23	2.02	0.41
1:A:86:LEU:HD13	1:A:92:ALA:HA	2.02	0.41
1:C:1006:LYS:HB3	1:C:1006:LYS:HE2	1.86	0.41
1:C:1317:GLU:HA	1:C:1372:GLY:O	2.21	0.41
1:A:107:VAL:O	1:A:107:VAL:HG13	2.21	0.41
1:C:1057:HIS:CE1	1:C:1068:ASN:HD21	2.38	0.41
1:C:1288:LEU:HD12	1:C:1289:ILE:H	1.86	0.41
1:B:541:PRO:HD2	1:B:545:TYR:CD2	2.55	0.41
1:A:254:LEU:HA	1:A:254:LEU:HD12	1.93	0.41
1:D:1504:SER:N	1:D:1517:HIS:CD2	2.89	0.41
1:A:359:TYR:N	1:A:359:TYR:HD1	2.19	0.41
1:B:557:HIS:CE1	1:B:568:ASN:ND2	2.89	0.41
1:C:1177:ARG:HH22	1:C:1183:VAL:HG23	1.86	0.41
1:A:45:TYR:CE2	1:A:49:CYS:SG	3.12	0.41
1:D:1608:LEU:HD12	1:D:1608:LEU:HA	1.92	0.41
1:B:862:GLU:HG3	1:B:863:GLU:H	1.83	0.41
1:B:891:GLN:NE2	1:B:895:LYS:NZ	2.69	0.41
1:A:3:GLY:C	1:A:17:HIS:HD2	2.24	0.41
1:C:1093:ILE:HD13	1:C:1117:THR:HB	2.02	0.41
1:A:7:LEU:HD23	3:A:509:HOH:O	2.20	0.41
1:B:863:GLU:HA	1:B:866:HIS:CB	2.43	0.41
1:A:243:THR:CG2	1:A:245:ALA:H	2.34	0.41
1:D:1773:ALA:CB	1:D:1878:VAL:HG11	2.49	0.41
1:C:1329:MET:CE	1:C:1374:VAL:HB	2.48	0.41
1:A:204:LEU:HD23	1:A:226:GLY:HA3	2.02	0.41
1:C:1004:SER:O	1:C:1005:ASN:C	2.60	0.40
1:D:1804:ARG:NH2	3:D:1943:HOH:O	2.55	0.40
1:A:93:ILE:HD12	1:A:97:LEU:CD2	2.50	0.40
1:A:301:THR:O	1:A:305:GLN:CG	2.70	0.40
1:B:825:GLY:O	1:B:829:MET:HG2	2.21	0.40
1:C:1007:LEU:HD13	1:C:1007:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1340:SER:N	2:C:1400:SO4:O1	2.43	0.40
1:A:6:LYS:O	1:A:7:LEU:C	2.60	0.40
1:B:520:ASP:HB3	1:B:523:ASP:OD2	2.21	0.40
1:C:1341:LEU:CD1	1:C:1341:LEU:N	2.84	0.40
1:D:1823:GLY:HA2	1:D:1826:ARG:NH2	2.36	0.40
1:D:1839:VAL:O	1:D:1840:SER:HB2	2.21	0.40
1:B:504:SER:O	1:B:513:ARG:HD3	2.21	0.40
1:D:1655:TYR:CD1	1:D:1684:VAL:HG22	2.56	0.40
1:A:38:PHE:HA	1:D:1526:GLY:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/398 (99%)	380 (96%)	12 (3%)	3 (1%)	27	8
1	B	395/398 (99%)	373 (94%)	15 (4%)	7 (2%)	13	1
1	C	395/398 (99%)	378 (96%)	14 (4%)	3 (1%)	27	8
1	D	395/398 (99%)	375 (95%)	17 (4%)	3 (1%)	27	8
All	All	1580/1592 (99%)	1506 (95%)	58 (4%)	16 (1%)	22	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	862	GLU
1	C	1181	ALA
1	B	504	SER
1	C	1006	LYS
1	D	1821	GLY
1	A	240	LYS
1	A	340	SER
1	B	506	LYS
1	B	840	SER

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Mol	Chain	Res	Type
1	C	1005	ASN
1	D	1503	GLY
1	D	1840	SER
1	B	861	PRO
1	B	507	LEU
1	A	7	LEU
1	B	502	HIS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/306 (100%)	262 (86%)	44 (14%)	5	0
1	B	306/306 (100%)	261 (85%)	45 (15%)	4	0
1	C	306/306 (100%)	274 (90%)	32 (10%)	10	2
1	D	306/306 (100%)	277 (90%)	29 (10%)	12	2
All	All	1224/1224 (100%)	1074 (88%)	150 (12%)	7	1

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	HIS
1	A	5	ASN
1	A	7	LEU
1	A	66	THR
1	A	84	LEU
1	A	93	ILE
1	A	97	LEU
1	A	99	THR
1	A	106	GLU
1	A	111	ASN
1	A	131	LYS
1	A	132	LEU
1	A	135	VAL
1	A	140	LEU

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Mol	Chain	Res	Type
1	A	141	GLN
1	A	152	ARG
1	A	177	ARG
1	A	213	LEU
1	A	230	LEU
1	A	240	LYS
1	A	243	THR
1	A	263	ASN
1	A	264	LEU
1	A	268	ARG
1	A	275	VAL
1	A	280	LEU
1	A	305	GLN
1	A	314	ILE
1	A	317	GLU
1	A	319	LYS
1	A	322	ILE
1	A	333	GLN
1	A	334	LEU
1	A	341	LEU
1	A	345	GLU
1	A	347	LEU
1	A	358	SER
1	A	362	GLU
1	A	373	LEU
1	A	374	VAL
1	A	383	ILE
1	A	391	GLN
1	A	397	SER
1	B	502	HIS
1	B	504	SER
1	B	507	LEU
1	B	544	GLU
1	B	553	GLU
1	B	569	LEU
1	B	570	LEU
1	B	584	LEU
1	B	599	THR
1	B	608	LEU
1	B	609	LEU
1	B	621	LEU
1	B	625	ILE

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Mol	Chain	Res	Type
1	B	633	ARG
1	B	643	LEU
1	B	652	ARG
1	B	663	ASN
1	B	677	ARG
1	B	678	LYS
1	B	684	VAL
1	B	698	LEU
1	B	700	LEU
1	B	704	LEU
1	B	705	VAL
1	B	713	LEU
1	B	730	LEU
1	B	736	LEU
1	B	755	LEU
1	B	768	ARG
1	B	776	LEU
1	B	789	ILE
1	B	794	LEU
1	B	802	LEU
1	B	805	GLN
1	B	814	ILE
1	B	841	LEU
1	B	845	GLU
1	B	857	SER
1	B	860	THR
1	B	862	GLU
1	B	863	GLU
1	B	887	LEU
1	B	891	GLN
1	B	894	LEU
1	B	895	LYS
1	C	1001	MET
1	C	1002	HIS
1	C	1005	ASN
1	C	1007	LEU
1	C	1015	ILE
1	C	1028	LEU
1	C	1093	ILE
1	C	1099	THR
1	C	1108	LEU
1	C	1117	THR

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Mol	Chain	Res	Type
1	C	1125	ILE
1	C	1132	LEU
1	C	1140	LEU
1	C	1143	LEU
1	C	1152	ARG
1	C	1174	LYS
1	C	1177	ARG
1	C	1214	SER
1	C	1219	ILE
1	C	1239	LEU
1	C	1243	THR
1	C	1254	LEU
1	C	1262	LEU
1	C	1264	LEU
1	C	1285	GLN
1	C	1317	GLU
1	C	1322	ILE
1	C	1341	LEU
1	C	1358	SER
1	C	1364	ARG
1	C	1376	LEU
1	C	1395	LYS
1	D	1501	MET
1	D	1506	LYS
1	D	1507	LEU
1	D	1522	GLN
1	D	1542	THR
1	D	1554	GLN
1	D	1573	ARG
1	D	1599	THR
1	D	1601	LEU
1	D	1608	LEU
1	D	1632	LEU
1	D	1641	GLN
1	D	1652	ARG
1	D	1653	VAL
1	D	1674	LYS
1	D	1678	LYS
1	D	1684	VAL
1	D	1730	LEU
1	D	1739	LEU
1	D	1776	LEU

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Mol	Chain	Res	Type
1	D	1802	LEU
1	D	1840	SER
1	D	1841	LEU
1	D	1873	LEU
1	D	1886	LEU
1	D	1887	LEU
1	D	1892	GLN
1	D	1894	LEU
1	D	1895	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	17	HIS
1	A	68	ASN
1	A	111	ASN
1	A	134	HIS
1	A	207	HIS
1	A	250	HIS
1	A	263	ASN
1	A	274	GLN
1	A	283	GLN
1	A	309	GLN
1	A	333	GLN
1	B	522	GLN
1	B	524	HIS
1	B	557	HIS
1	B	564	ASN
1	B	568	ASN
1	B	641	GLN
1	B	663	ASN
1	B	679	HIS
1	B	707	HIS
1	B	728	GLN
1	B	774	GLN
1	B	790	HIS
1	B	799	GLN
1	B	830	ASN
1	B	891	GLN
1	C	1005	ASN
1	C	1034	GLN

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Mol	Chain	Res	Type
1	C	1057	HIS
1	C	1068	ASN
1	C	1141	GLN
1	C	1165	HIS
1	C	1187	ASN
1	C	1237	GLN
1	C	1250	HIS
1	C	1274	GLN
1	C	1285	GLN
1	C	1290	HIS
1	C	1299	GLN
1	C	1306	GLN
1	C	1309	GLN
1	C	1349	GLN
1	D	1517	HIS
1	D	1522	GLN
1	D	1524	HIS
1	D	1534	GLN
1	D	1568	ASN
1	D	1611	ASN
1	D	1641	GLN
1	D	1663	ASN
1	D	1687	ASN
1	D	1695	GLN
1	D	1707	HIS
1	D	1774	GLN
1	D	1790	HIS
1	D	1830	ASN
1	D	1892	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	LLP	A	211	1	24,24,25	4.46	7 (29%)	30,32,34	1.46	4 (13%)
1	LLP	B	711	1	24,24,25	4.24	6 (25%)	30,32,34	1.45	3 (10%)
1	LLP	C	1211	1	24,24,25	4.13	7 (29%)	30,32,34	1.40	4 (13%)
1	LLP	D	1711	1	24,24,25	4.37	6 (25%)	30,32,34	1.43	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	211	1	-	0/15/17/19	0/1/1/1
1	LLP	B	711	1	-	0/15/17/19	0/1/1/1
1	LLP	C	1211	1	-	0/15/17/19	0/1/1/1
1	LLP	D	1711	1	-	0/15/17/19	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	LLP	O-C	18.62	1.24	1.11
1	D	1711	LLP	O-C	17.98	1.23	1.11
1	B	711	LLP	O-C	17.23	1.23	1.11
1	C	1211	LLP	O-C	16.66	1.22	1.11
1	B	711	LLP	C6-C5	6.61	1.53	1.37
1	D	1711	LLP	C6-C5	6.54	1.53	1.37
1	C	1211	LLP	C6-C5	6.52	1.53	1.37
1	A	211	LLP	C6-C5	6.38	1.52	1.37
1	B	711	LLP	C6-N1	5.52	1.46	1.34
1	C	1211	LLP	O3-C3	-5.46	1.23	1.37
1	B	711	LLP	O3-C3	-5.40	1.24	1.37
1	D	1711	LLP	C6-N1	5.33	1.46	1.34
1	A	211	LLP	O3-C3	-5.32	1.24	1.37
1	C	1211	LLP	C6-N1	5.32	1.46	1.34
1	D	1711	LLP	O3-C3	-5.27	1.24	1.37
1	A	211	LLP	C6-N1	5.21	1.46	1.34
1	A	211	LLP	P-OP4	-3.23	1.48	1.60
1	D	1711	LLP	P-OP4	-3.19	1.49	1.60
1	D	1711	LLP	CA-C	3.04	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1211	LLP	P-OP4	-2.97	1.49	1.60
1	A	211	LLP	CA-C	2.95	1.53	1.48
1	B	711	LLP	P-OP4	-2.92	1.50	1.60
1	B	711	LLP	CA-C	2.80	1.53	1.48
1	C	1211	LLP	CA-C	2.45	1.52	1.48
1	C	1211	LLP	P-OP2	-2.01	1.47	1.54
1	A	211	LLP	P-OP2	-2.00	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LLP	C5-C6-N1	-5.57	113.81	123.86
1	D	1711	LLP	C5-C6-N1	-5.49	113.97	123.86
1	B	711	LLP	C5-C6-N1	-5.44	114.06	123.86
1	C	1211	LLP	C5-C6-N1	-5.32	114.26	123.86
1	A	211	LLP	C6-C5-C4	2.95	120.34	118.10
1	C	1211	LLP	C6-C5-C4	2.70	120.15	118.10
1	D	1711	LLP	C6-C5-C4	2.61	120.08	118.10
1	B	711	LLP	C6-C5-C4	2.43	119.95	118.10
1	D	1711	LLP	C2'-C2-C3	-2.36	118.15	121.02
1	B	711	LLP	C2'-C2-C3	-2.26	118.27	121.02
1	A	211	LLP	C6-N1-C2	2.09	123.76	119.28
1	A	211	LLP	C4'-NZ-CE	2.07	121.09	113.47
1	C	1211	LLP	C4'-NZ-CE	2.02	120.90	113.47
1	C	1211	LLP	C2'-C2-C3	-2.01	118.56	121.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	400	-	4,4,4	0.79	0	6,6,6	0.09	0
2	SO4	B	900	-	4,4,4	0.52	0	6,6,6	0.06	0
2	SO4	C	1400	-	4,4,4	0.60	0	6,6,6	0.08	0
2	SO4	D	1900	-	4,4,4	0.61	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	400	-	-	0/0/0/0	0/0/0/0
2	SO4	B	900	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1400	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1900	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.